PARAMETER ESTIMATION AND THE USE OF CATALOG DATA WITH TRNSYS

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ABSTRACT

General models for heat and mass transfer components have been developed for use in TRNSYS [1] thermal system simulations. These components remove some of the idealizations and detailed specifications that are required in existing TRNSYS component models. In these new component formulations, a set of parameters characterizing the performance of the component are fit using catalog data.

This paper presents a technique for parameter estimation that can be used with realistic models to accurately represent equipment performance. The new models are formulated for three heat and mass transfer devices: sensible heat exchangers, chilled water cooling coils, and direct expansion cooling coils. The performance of the components using the parameter estimation routine is evaluated.

INTRODUCTION

TRNSYS is a transient system simulation program consisting of individual component models that are connected by the user in order to simulate the performance of a complete thermal system. Two such current component models are the Type 5 Heat Exchanger and the Type 52 Cooling Coil.

The Type 5 and Type 52 components are excellent examples for illustrating the goal of this project. These two components contain assumptions and require parameters that make it difficult to replicate cataloged performance. The Type 5 Heat Exchanger uses either a constant effectiveness or a constant overall heat transfer coefficient. However, these two parameters are really both functions of the fluid properties and the mass flow rate. The Type 52 Cooling Coil requires geometric parameters such as fin thickness and the water tube spacing both parallel and perpendicular to the air flow. Including the effects of flow rate would require detailed modeling.

A new method has been devised for modeling the performance of real components while avoiding many simplifying assumptions and the complications of requiring detailed specifications. This method is based on fundamental heat and mass transfer correlations that are manipulated so that all geometric terms are lumped into parameters that are then fit using catalog data. It is assumed the component itself has zero thermal capacitance, and the models are therefore steady-state. Component performance can then be predicted using the flow rates, fluid properties, and fitted parameters. This method has been successfully applied to sensible heat exchangers, chilled water cooling coils, and direct expansion cooling coils.

SENSIBLE HEAT EXCHANGER MODEL

A sensible heat exchanger model has been developed for shell and tube heat exchangers, radiators, and similar geometries in which the inner fluid flows through tubes while the outer fluid flows perpendicular to the tube bank. This model is based on fundamental correlations for both heat transfer and pressure drop.

Heat Transfer

The overall heat transfer coefficient is based on two heat transfer resistances in series: the heat transfer resistance between the inner fluid and the tube wall, and the heat transfer resistance between the tube/fin surface and the outer fluid. The heat transfer coefficient between the tube/fin surface and the outer fluid is based on the correlation of Zhukauskas [2]:

$$\overline{Nu}_D = C\, Re_{D,\,max}^{m}\, Pr^{0.36} \left(\frac{Pr}{Pr_s}\right)^{1/4} \qquad (1)$$

The heat transfer coefficient between the inner fluid and the tube wall is based on the Sieder-Tate equation [2], which is similar to the familiar Dittus-Boelter equation:

$$Nu_D = 0.027\, Re_D^{4/5}\, Pr^{1/3} \left(\frac{\mu}{\mu_s}\right)^{0.14} \qquad (2)$$

Equations 1 and 2 are modified by introducing unknown parameters to account for geometric considerations such as flow areas, surface areas, and tube bank arrangement, as well as an assumed constant fin efficiency. Equations 1 and 2 are generalized to yield Equations 3-5:

$$(hA)_o = C_1\left(\frac{m_o}{\mu_o}\right)^{C_2} Pr_o^{0.36}\left(\frac{Pr_o}{Pr_{o,s}}\right)^{1/4} k_o \quad (3)$$

$$(hA)_i = C_3\left(\frac{m_i}{\mu_i}\right)^{4/5} Pr_i^{1/3}\left(\frac{\mu_i}{\mu_{i,s}}\right)^{0.14} k_i \quad (4)$$

$$(UA)_{tot} = \frac{1}{\frac{1}{(hA)_o} + \frac{1}{(hA)_i}} \quad (5)$$

The values of the three performance parameters C_1, C_2, and C_3 need to be fit using catalog data.

In fitting these parameters with catalog data, two important issues need to be resolved: the number of data points required for a good fit of the parameters, and the means by which these data points are chosen. It has been found that at least 16 data points are required to provide a good fit. Using more than 16 data points results in little improvement in the average error and bias of the calculated heat transfer rate. These data points need to be chosen to provide all combinations of high and low values of the four operational parameters: tube fluid mass flow rate, shell fluid mass flow rate, tube fluid inlet temperature, and shell fluid inlet temperature. Choosing data points in this way yields a good fit because it covers the entire operating range and results in a wide range of values for the two heat transfer resistances. This improves the accuracy of determining the parameter values.

Figures 1 and 2 illustrate the parameter estimation applied to the catalog data of a single-pass shell and tube heat exchanger [3]. The shell fluid is SAE-10 oil, and the tube fluid is water. The parameter fitting and plotting were performed by the Engineering Equation Solver (EES) software package [4]. In the figures shown in this paper, the data points used to fit the parameters are shown by the larger, filled symbols. It can be seen that the 16 fitting data points do indeed cover the entire operating range.

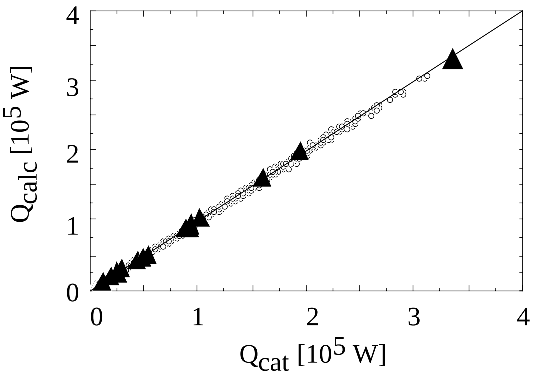


Figure 1. Calculated heat transfer rate vs. catalog heat transfer rate for the sensible heat exchanger model.

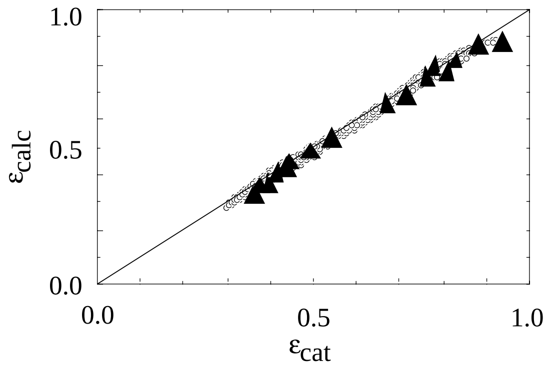


Figure 2. Calculated effectiveness vs. catalog effectiveness for the sensible heat exchanger model.

The three parameters used to generate Figures 1 and 2 were fitted by minimizing the sum of the squares of the errors between the calculated heat transfer rate and the catalog heat transfer rate. Effectiveness was calculated as a secondary quantity. The RMS error in the heat transfer rate is 1829 W (about 1%), and the RMS error in the effectiveness is 0.01. The agreement between the calculated effectiveness and the catalog effectiveness indicates the accuracy of the property correlations.

Pressure Drop

The new sensible heat exchanger model also predicts the pressure drop of each fluid. For turbulent flow, the tube fluid friction factor is based on a correlation approximating the smooth surface condition of the Moody diagram [2]:

$$f = 0.316\ Re_D^{-1/4} \quad (6)$$

The shell fluid pressure drop assumes a power relationship between the friction factor and the shell fluid Reynolds number [5].

$$f \propto Re_{D,\,max}^{C} \quad (7)$$

Generalizing the equations by introducing unknown parameters results in Equations 8 and 9.

$$\Delta P_o = C_4 \left(\frac{m_o}{\mu_o}\right)^{C_5} \left(\frac{m_o^2}{\rho_o}\right) \tag{8}$$

$$\Delta P_i = C_6 \left(\frac{m_i}{\mu_i}\right)^{-1/4} \left(\frac{m_i^2}{\rho_i}\right) \left(\frac{\mu_i}{\mu_{i,s}}\right)^{0.14} \tag{9}$$

SENSIBLE HEAT EXCHANGER TRNSYS COMPONENT

A TRNSYS component has been written that uses the fitted performance parameters to predict the heat exchanger performance in simulations. In addition to the fitted parameters, the TRNSYS component requires parameters to indicate which fluids are flowing through the heat exchanger as well as their compositions, if applicable (e.g. grade of SAE oil or percent ethylene glycol in a water/ethylene glycol solution).

CHILLED WATER COOLING COIL MODEL

Two models similar to that of the sensible heat exchanger have been developed for chilled water cooling coils. Both of these models use the heat exchanger analogy method [6].

A simple model for a cooling coil is based on the heat exchanger analogy method, which allows a wet cooling coil to be analyzed using the effectiveness-Ntu heat exchanger equations based on enthalpy rather than temperature. Analogous to the capacitance rates C_{min} and C_{max} and the capacitance rate ratio C^* used in heat exchanger analysis, the heat exchanger analogy method uses mass capacitance rates m_{min} and m_{max} and a mass capacitance rate ratio m^* as given by Equation 10. Using the saturation specific heat $c_{p,\,sat}$ defined by Equation 11, the liquid mass flow rate is converted to an equivalent flow rate of saturated air.

$$m^* = \frac{\min\left[m_o,\ m_i\left(\frac{c_{p,\,i}}{c_{p,\,sat}}\right)\right]}{\max\left[m_o,\ m_i\left(\frac{c_{p,\,i}}{c_{p,\,sat}}\right)\right]} \tag{10}$$

$$c_{p,\,sat} = \frac{h_{sat}\big|_{T=EDP} - h_{sat}\big|_{T=EWT}}{EDP - EWT} \tag{11}$$

At this point, the Ntu value is calculated using the minimum mass capacitance rate and the overall enthalpy transfer coefficient-area product defined by Equation 12.

$$UA_{enthalpy} = \frac{1}{\frac{c_{p,\,o}}{(\bar{h}\,A)_o} + \frac{c_{p,\,sat}}{(h\,A)_i}} \tag{12}$$

The effectiveness is calculated using the Ntu value and the mass capacitance rate ratio, and the maximum heat transfer rate is calculated using the effectiveness, the minimum mass capacitance rate, the air inlet enthalpy, and the saturation enthalpy of air at the entering liquid temperature. The exit air enthalpy can then be determined. To calculate the exit air temperature, the air stream and the condensate film (assumed to be at a constant temperature along the entire coil surface) are treated as a sensible heat exchanger with a capacitance rate ratio of zero.

In the simple chilled water cooling coil model, the coil is treated as being either totally dry or totally wet. For totally dry operation, the model is identical to that of the sensible heat exchanger (Equations 3-5). For totally wet operation, the air side heat transfer coefficient-area product includes a correction factor based on the air velocity [7] as shown in Equations 13 and 14.

$$(hA)_o = C_f\, C_1 \left(\frac{m_o}{\mu_o}\right)^{C_2} Pr_o^{0.36} \left(\frac{Pr_o}{Pr_{o,\,s}}\right)^{1/4} k_o \tag{13}$$

$$C_f = 0.626\ V_{std}^{0.101} \tag{14}$$

Figures 3-5 illustrate the performance of this simple cooling coil model determined from the parameter estimation technique compared to the catalog data. The relevant outputs are the heat transfer rate and the leaving dry bulb and wet bulb temperatures.

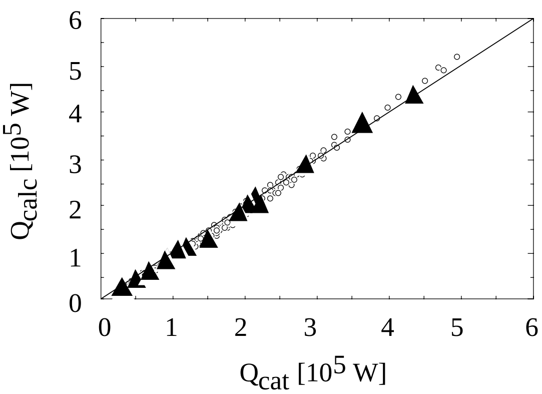


Figure 3. Calculated heat transfer rate vs. catalog heat transfer rate for the simple cooling coil model.

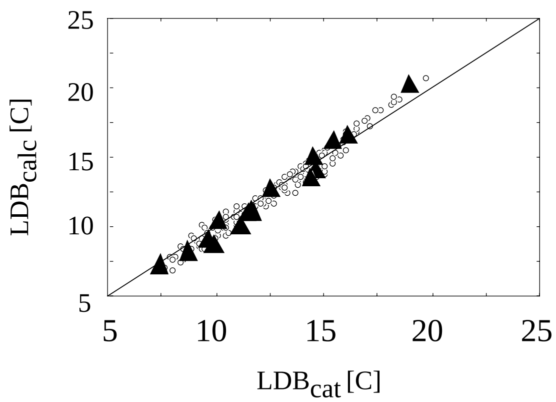


Figure 4. Calculated leaving dry bulb temperature vs. catalog leaving dry bulb temperature for the simple cooling coil model.

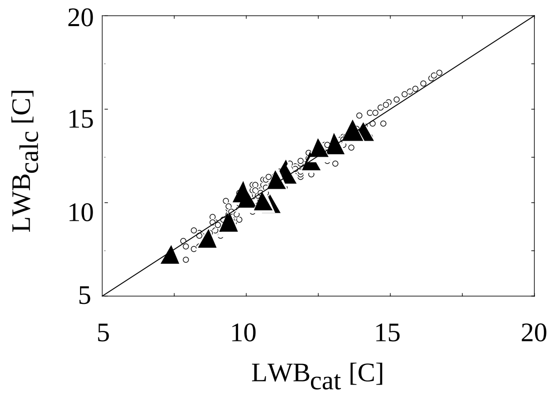


Figure 5. Calculated leaving wet bulb temperature vs. catalog leaving wet bulb temperature for the simple cooling coil model.

The RMS error in the heat transfer rate is 10294 W, or about 3.5%. The RMS error in the leaving dry bulb temperature is 0.56 C, and the RMS error in the leaving wet bulb temperature is 0.40 C. The greater error in the dry bulb temperature results from the assumption of a constant condensate temperature throughout the coil.

In simulating coil performance, the heat transfer rate is calculated for both totally dry and totally wet operation. A comparison is then made to determine which operating condition better approximates the actual operating condition. If the entering air dew point temperature is lower than the entering liquid temperature, the coil is totally dry. If the entering air dew point temperature is higher than the tube surface temperature at the entrance, the coil is totally wet. Otherwise, the coil is partially wet. In this case, the coil is approximated as being either totally wet or totally dry, whichever yields the higher heat transfer rate. This is done because modeling the coil as either totally dry or totally wet underestimates the actual heat transfer rate. Assuming totally dry operation neglects latent heat transfer. Assuming totally wet operation requires humidification of the air so that condensation will occur over the entire coil surface. The heat transfer to the air in order to maintain its dry bulb temperature as this 'artificial' moisture is added reduces the calculated net heat transfer rate from the air.

The detailed model of the chilled water cooling coil is different from the simple model in that it calculates the fraction of the coil surface that is wet rather than assuming it is either totally dry or totally wet. The total coil is analyzed as a dry coil in series with a wet coil. In this model, two sets of parameters are required: one set fit to totally dry operating points and another set fit to totally wet operating points. Differences in the two sets of parameters result from assumptions in the wet coil model, such as a constant condensate temperature. These parameters, along with the calculated fraction of the coil surface that is wet, result in Equations 15-18.

$$(hA)_{o,d} = (1 - f_w) C_{1,d} \left(\frac{m_o}{\mu_o} \right)^{C_{2,d}} Pr_o^{0.36} \left(\frac{Pr_o}{Pr_{o,s}} \right)^{1/4} k_o \tag{15}$$

$$(hA)_{i,d} = (1 - f_w) C_{3,d} \left(\frac{m_i}{\mu_i} \right)^{4/5} Pr_i^{1/3} \left(\frac{\mu_i}{\mu_{i,s}} \right)^{0.14} k_i \tag{16}$$

$$(hA)_{o,w} = f_w C_f C_{1,w} \left(\frac{m_o}{\mu_o} \right)^{C_{2,w}} Pr_o^{0.36} \left(\frac{Pr_o}{Pr_{o,s}} \right)^{1/4} k_o \tag{17}$$

$$(hA)_{i,w} = f_w C_{3,w} \left(\frac{m_i}{\mu_i} \right)^{4/5} Pr_i^{1/3} \left(\frac{\mu_i}{\mu_{i,s}} \right)^{0.14} k_i \tag{18}$$

Figure 6 illustrates how well these parameters can be fit to predict totally dry operation of the coil. Similar results are seen when parameters are fit to predict totally wet operation of the coil.

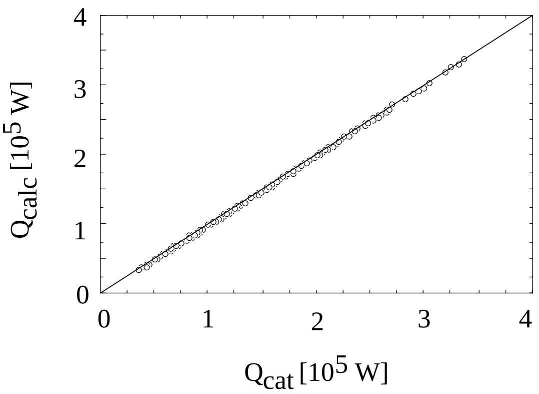


Figure 6. Calculated heat transfer rate vs. catalog heat transfer rate for totally dry operation.

Iterating on both the liquid temperature at the wet/dry boundary and the wet fraction of the coil surface results in the excellent agreement between predicted and cataloged results seen in Figure 7.

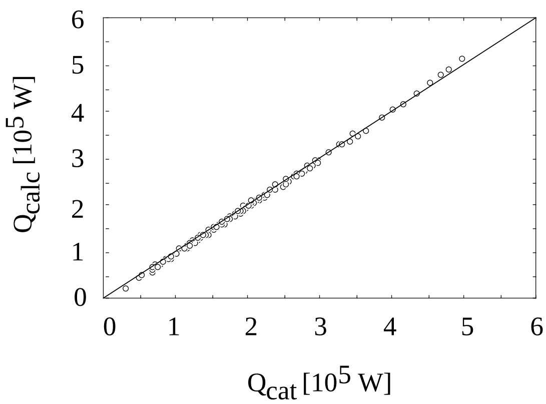


Figure 7. Calculated heat transfer rate vs. catalog heat transfer rate for partially wet operation.

The RMS error in the heat transfer rate is 4108 W (about 1.4%), the RMS error in the leaving dry bulb temperature is 0.46 C, and the RMS error in the leaving wet bulb temperature is 0.16 C. These statistics all show a significant improvement in accuracy over that of the simple model.

DIRECT EXPANSION COOLING COIL MODEL-HEAT TRANSFER

A direct expansion cooling coil model has been developed that is similar to the simple chilled water cooling coil model in that the coil surface is treated as either totally dry or totally wet. The air side heat transfer correlations are identical to those of the chilled water cooling coil model (Equation 3 for totally dry operation and Equations 13 and 14 for totally wet operation). Due to the complexity and case-dependency of most boiling heat transfer correlations, the refrigerant boiling heat transfer correlation of Equation 19 is based on a manufacturer's correlation fit to experimental data. It is similar to the correlation of Pierre [8].

$$(hA)_i = C_3 \, k_{ref,\,l} \left(\frac{m_{ref}}{\mu_{ref,\,l}} \, \Delta h \right)^{0.45} \qquad (19)$$

Figure 8 illustrates the generally good agreement between the predicted and the cataloged operational points. The RMS error in the heat transfer rate is 222 W (about 2.2%), the RMS error in the leaving dry bulb temperature is 0.36 C, and the RMS error in the leaving wet bulb temperature is 0.32 C.

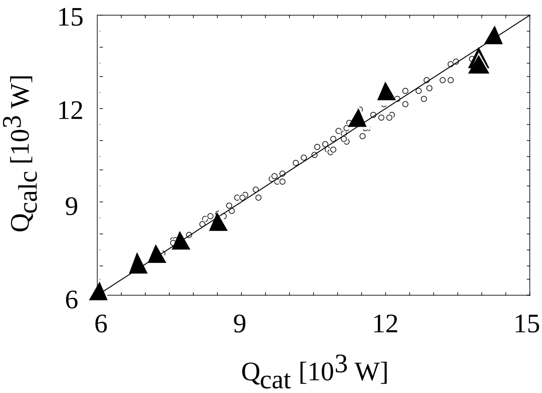


Figure 8. Calculated heat transfer rate vs. catalog heat transfer rate for an R-12 direct expansion cooling coil.

EXTENSION OF PARAMETERS TO OPERATION WITH OTHER FLUIDS

An important objective of this project is to create general component models that will allow performance prediction with any fluids. For this reason, all of the equations cited within this paper retain all transport properties such as dynamic viscosity and thermal conductivity. Only geometric terms and a constant fin efficiency are lumped into the fitted parameters. As a result, the fitted parameters should be valid for a given component from a manufacturer's catalog regardless of what fluids are used.

To test the applicability of the fitted parameters to other fluids, operating points for a shell and tube heat exchanger with three different shell fluids have been obtained from the manufacturer. The three shell fluids are water, a 50% ethylene glycol/water solution, and SAE-10 oil. The tube fluid is water in all three cases.

Table 1 lists the errors in the calculated heat transfer rate, compared to the cataloged heat transfer rate, that result when the fitted parameters are applied to each of the fluid combinations. The first column indicates the shell fluid for which the parameters are fit. The three following columns indicate the shell fluid to which the parameters are applied. In general, the model performs well when the parameters fit with one set of fluids are applied to a different set of fluids.

Table 1. Results of applying fitted parameters to heat exchanger operation with other fluids.

Fit fluid	Avg. % error when applied to: H_2O	50% EG	SAE 10
H_2O	0.79	3.28	18.98
50% EG	0.90	0.80	5.28
SAE 10	2.69	1.90	3.99

The errors result from several sources. One source is the transport property correlations. Whenever possible, published correlations are used. In some cases however, only data points are available and a curve fit is required. A second source of error is that the fin efficiency is assumed constant. The fin efficiency is a function of the fluid transport properties, and so some error will result when the fitted parameters are applied to various fluids. The shell fluid Reynolds number exponent is also a source of error. This exponent is a function of the Reynolds number itself, and therefore it would be expected to vary with different fluids. Finally, errors result due to differences between this model and the manufacturer's model used to generate catalog data.

In a cooling coil, fluids such as ethylene glycol/water and calcium chloride/water may be used instead of chilled water. Figures 9 and 10 illustrate the performance of the simple and detailed models, respectively, when the parameters fitted with a chilled water coil are applied to the same coil using a 50% ethylene glycol/water solution.

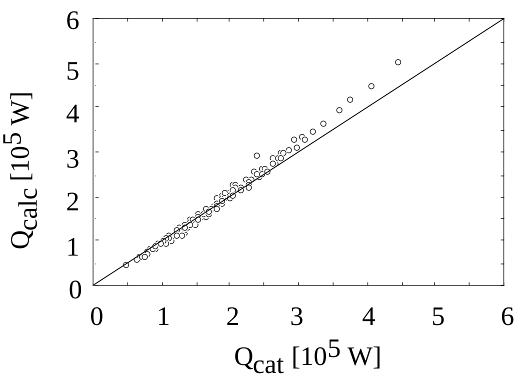


Figure 9. Calculated heat transfer rate vs. catalog heat transfer rate for the simple cooling coil model.

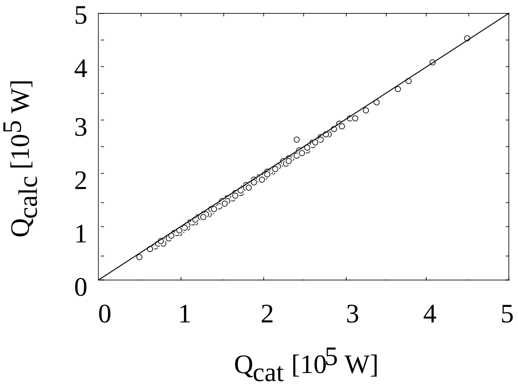


Figure 10. Calculated heat transfer rate vs. catalog heat transfer rate for the detailed cooling coil model.

Sources of error include those previously mentioned as well as errors resulting from assumptions used in the heat exchanger analogy method, such as the assumption of a constant condensate temperature throughout the coil.

Direct expansion cooling coils may use a variety of refrigerants. However, most catalog data are based on operation with either R-12 or R-22. Figure 11 illustrates the predictive capability of the model when parameters fit using R-12 operating points are applied to operating points using R-22.

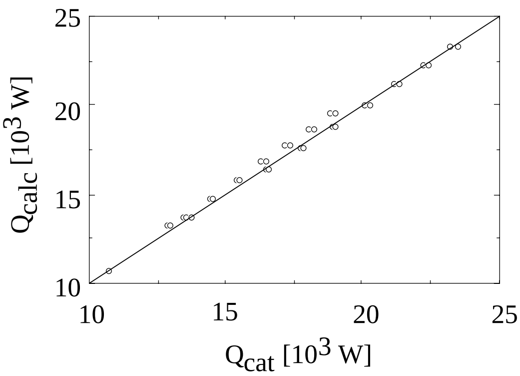
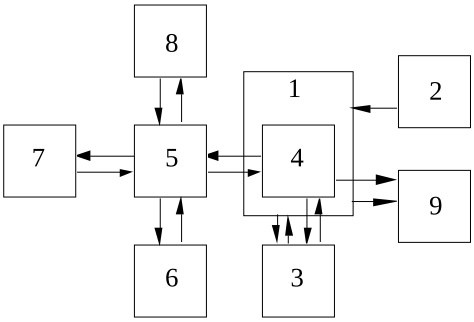


Figure 11. Calculated heat transfer rate vs. catalog heat transfer rate for an R-22 direct expansion cooling coil.

PARAMETER ESTIMATION

In all of the simulations previously shown, the parameter estimation was performed using the EES software package. To use these new component models in thermal system simulations, the parameter estimation must be moved into an environment that can be used in conjunction with TRNSYS. This is being accomplished using the IMSL routine DBCONF. This optimization routine uses a quasi-Newton method and a finite-difference gradient to minimize a function with simple bounds on the variables. Figure 12 is a schematic showing how this routine is used to perform the parameter estimation.



1. Main program
2. Data file
3. IMSL routine DBCONF
4. Subroutine ERRCALC
5. TRNSYS Type
6. Subroutine NEWFLUIDS
7. Subroutine REFTRANS
8. TRNSYS utilities
9. Output files

Figure 12. Schematic of the parameter estimation method to be used in conjunction with TRNSYS.

The main program reads the performance data from the data file, calculates guess values for the parameters, writes some output files, and performs any required initializations. The main program calls the DBCONF routine, which in turn calls the subroutine ERRCALC. Subroutine ERRCALC calls the TRNSYS component of interest to calculate the component performance using inputs from the data file and the parameters from the DBCONF routine. The TRNSYS component may use the subroutines NEWFLUIDS (transport properties of non-refrigerant fluids) and REFTRANS (transport properties of saturated liquid refrigerants), and possibly some TRNSYS utilities such as PSYCH (psychrometrics) and FLUIDS (thermodynamic properties of refrigerants). Subroutine ERRCALC then calculates the total error between the calculated component performance and the catalog performance from the data file. DBCONF then adjusts the parameters. This process is repeated until the sum of the squares of the errors is minimized. More output files are then created to give the final parameter values and to compare the calculated performance with the catalog performance at these final parameter values.

Initial results of this parameter estimation method are encouraging. The results of the DBCONF parameter estimation routine results are in good agreement with those of EES.

CONCLUSIONS

New component models have been written to allow catalog data to be used with TRNSYS. Based on fundamental heat and mass transfer relations, these models include parameters whose values are determined using catalog data. Because all fluid properties are retained in the heat and mass transfer relations, the parameters are functions only of geometry. These parameters allow cataloged components for which either detailed geometric specifications or performance data for the fluids of interest are not readily available to be used in TRNSYS thermal system simulations.

This new method of component modeling offers additional advantages over existing models. In contrast to existing simple models, these new models require only a small number of parameter values to be fit simultaneously. Simplifying assumptions such as a constant heat exchanger effectiveness are also not used. In contrast to existing detailed models, the new models require few geometric specifications. The sensible heat exchanger model requires no geometric specifications while the cooling coil models require only the coil face area.

The models and fitted parameters replicate the performance of sensible heat exchangers, chilled water cooling coils, and direct expansion cooling coils quite accurately. The parameter fitting routine is general and applicable to a wide variety of components. It is anticipated that this method will be applied to additional heat and mass transfer devices and possibly to other components and subsystems.

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NOMENCLATURE

EES programs were written in English units in order to simplify use of the manufacturers' catalogs. The TRNSYS components and associated subroutines use SI units.

C	Parameter
C_f	Wet surface convection coefficient correction factor
$c_{p,\,i}$	Specific heat of inner fluid (kJ/kg-C, Btu/lbm-F)
$c_{p,\,o}$	Specific heat of outer fluid (kJ/kg-C, Btu/lbm-F)
$c_{p,\,sat}$	Saturation specific heat (kJ/kg-C, Btu/lbm-F)
Δh	Enthalpy change (kJ/kg, Btu/lbm)
ΔP	Pressure drop (kPa, psi)
EDP	Entering dew point temperature (C, F)
EWT	Entering water temperature (C, F)
f_w	Wet fraction of coil surface
h	Enthalpy (kJ/kg, Btu/lbm)
hA	Convection coefficient-area product (kJ/hr-C, Btu/hr-F, Btu/min-F)
k	Thermal conductivity (W/m-K, Btu/hr-ft-F)
LDB	Leaving dry bulb temperature (C, F)
LWB	Leaving wet bulb temperature (C, F)
m	Mass flow rate (kg/hr, lbm/hr, lbm/min)
m^*	Mass capacitance rate ratio
μ	Dynamic viscosity (Pa-s, lbm/ft-hr)
Ntu	Number of transfer units
Nu	Nusselt number
Pr	Prandtl number
Q	Heat transfer rate (kJ/hr, Btu/min, Btu/hr)
Re	Reynolds number
ρ	Density (kg/m^3, lbm/ft^3)
UA	Overall heat transfer coefficient-area product (kJ/hr-C, Btu/hr-F, Btu/min-F)
$UA_{enth.}$	Overall enthalpy transfer coefficient-area product (kg/hr, lbm/hr, lbm/min)
V	Face velocity (ft/min)

Subscripts

calc	Calculated value
cat	Catalog value
d	Totally dry operation
i	Inner fluid
l	Saturated liquid condition
o	Outer fluid
ref	Refrigerant
s	Surface condition
sat	Saturated
std	At standard conditions
tot	Total
w	Totally wet operation